

Heuristic theory for many-faced d -dimensional Poisson-Voronoi cells

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Abstract

We consider the d -dimensional Poisson-Voronoi tessellation and investigate the applicability of heuristic methods developed recently for two dimensions. Let $p_n(d)$ be the probability that a cell have n neighbors (be ‘ n -faced’) and $m_n(d)$ the average facedness of a cell adjacent to an n -faced cell. We obtain the leading order terms of the asymptotic large- n expansions for $p_n(d)$ and $m_n(3)$. It appears that, just as in dimension two, the Poisson-Voronoi tessellation violates Aboav’s ‘linear law’ also in dimension three. A confrontation of this statement with existing Monte Carlo work remains inconclusive. However, simulations upgraded to the level of present-day computer capacity will in principle be able to confirm (or invalidate) our theory.

Keywords: Poisson-Voronoi cell, number of neighbors, two-cell correlation, Aboav’s law

1 Introduction

1.1 General

Cellular structures occur in a wide variety of natural systems. The examples most quoted, but by no means the only ones, are soap froths and biological tissues. Cellular systems also serve as a tool of analysis in a diversity of problems throughout the sciences and beyond. Many references may be found in Okabe *et al.* [1], Rivier [2], and Hilhorst [3].

A popular model of a cellular structure is the Voronoi tessellation. It is obtained by performing the Voronoi construction on a set of point-like ‘seeds’ in d -dimensional space. This construction consists of partitioning space into cells in such a way that each point of space is in the cell of the seed to which it is closest. A d -dimensional Voronoi cell is convex and is bounded by planar $(d-1)$ -dimensional faces. Two cells are called ‘neighbors’ or ‘adjacent’ when they have a face in common. The Voronoi construction may thus serve to define neighbor relations on an arbitrary set of given seeds.

In the special case that the seed positions are drawn randomly from a uniform distribution, one speaks of the *Poisson*-Voronoi tessellation. It constitutes one of the simplest and best studied models of a cellular structure. The analytic study of the statistical properties of the Poisson-Voronoi tessellation in dimensions $d = 2, 3$ was initiated by Meijering [4] in 1953. Monte Carlo results were obtained by several workers in the past decades (see [1] for references). The analytical and numerical results of greatest interest in dimensions $d = 2$ and $d = 3$ have been listed in Ref. [1]. In arbitrary dimension d , a large collection of statistical properties of the Poisson-Voronoi tessellations were derived in Refs. [5, 6].

One of the most characteristic properties of a cell is its number n of faces, and it so happens that this is not a property easy to study analytically. There must be at least $d+1$ faces, but there may be any number of them. We denote by $p_n(d)$ the probability that a randomly picked cell (all cells with the same probability) be n -faced. The facedness probability $p_n(d)$ has been the center of interest of experimental and Monte Carlo work (see [1, 2, 3] for references), especially in $d = 2$ and $d = 3$. Analytical results for this quantity, however, are very scarce. Only the one-dimensional case with $p_n(1) = \delta_{n,2}$ is trivial. Known results in higher dimension include the *average* facedness $\langle n \rangle_d = \sum_n n p_n(d)$ in dimensions $d = 2, 3, 4$. Its values are $\langle n \rangle_2 = 6$, $\langle n \rangle_3 = 2 + 48\pi^2/35 = 15.535\dots$, and $\langle n \rangle_4 = 340/9 = 37.77\dots$ [7]. It has been determined numerically that the peaks of the distributions are at $n = 6$ for $d = 2$ and at $n = 15$ for $d = 3$; as n increases beyond the peak value, $p_n(d)$ decreases very rapidly to zero.

1.2 Recent work

Although in general dimension d one readily writes down an nd -dimensional integral for $p_n(d)$, the variables of integration are coupled in such a way that for all $d > 1$ this is a true many-particle problem. As a consequence, it has not been possible to determine the neighbor number probability $p_n(d)$ analytically. In dimension $d = 2$ progress was made, nevertheless, in Refs. [8, 3], where it was shown that in the limit $n \rightarrow \infty$ the sidedness probability $p_n(2)$ has the exact asymptotic behavior

$$p_n(2) = \frac{C}{4\pi^2} \frac{(8\pi^2)^n}{(2n)!} [1 + o(1)], \quad n \rightarrow \infty, \quad (1.1)$$

with $C = 0.344\,347\dots$. The collection of asymptotic results that include (1.1) required considerable calculational effort. Subsequently, however, heuristic arguments were developed [9] by which at least part of the same results can be derived more easily. We extend in this work these heuristic methods to higher dimensions.

The correlation between the neighbor numbers of adjacent cells is usually expressed in terms of the quantity $m_n(d)$, defined as the average facedness of a cell that is itself adjacent to an n -faced cell. Aboav's celebrated 'linear law' states that $nm_n(d) = an + b$ [10]. It holds within error bars, and with system-specific a and b , for many experimental cellular systems. In Ref. [11] it was demonstrated, however, that for the two-dimensional Poisson-Voronoi tessellation Aboav's law is in fact a linear approximation limited to small n values. The true asymptotic behavior appeared to be

$$m_n(2) = 4 + 3(\pi/n)^{1/2} + \dots, \quad n \rightarrow \infty, \quad (1.2)$$

and shows that $nm_n(2)$, instead of being linear, has a small downward curvature. In fact, this deviation from the linear law was known from Monte Carlo simulations [12, 13, 14]. In this paper we investigate how (1.2) is modified in dimension $d = 3$.

1.3 This work

This work continues a series of articles [8, 3, 11, 15, 16, 9] that deal with the properties of Voronoi tessellations. We consider here the question of what, if anything, may be learned in higher dimensions from the two-dimensional case. The answer is that the exact methods, as in so many other domains of physics, remain limited to two dimensions of space. However, we can apply to higher dimensions the heuristic methods that we developed [9] on the basis of the exact ones.

In this way we obtain first, in section 2, we obtain a formula for the large- n behavior of $p_n(d)$ in arbitrary space dimension d . The argument is

a fairly straightforward extension from the two-dimensional case [9]. Then, in section 3, we obtain a two-term asymptotic large- n expansion of m_n in dimension $d = 3$. Our key results are represented by equations (2.20) and (3.2), that are the higher-dimensional analogs to (1.1) and (1.2), respectively. One of our findings is that Aboav’s law fails also for the *three*-dimensional Poisson-Voronoi tessellation. In section 4 we compare our theoretical result for $m_n(3)$ to existing Monte Carlo work. We conclude in section 5.

2 Asymptotic large- n expression for $p_n(d)$

We consider a d -dimensional Poisson-Voronoi tessellation with seed density ρ . This density may be scaled to unity but we will keep it as a check on dimensional coherence. We select an arbitrary seed, let its position be the origin, and are interested in its Voronoi cell, to be referred to as the ‘central cell’. The central cell has the same statistical properties as any other cell. We set ourselves as a first purpose to determine the facedness probability $p_n(d)$ of this cell in the limit of large n .

2.1 The shell of first neighbor seeds

In the two-dimensional case the n -sided cell is known for large n to tend with probability 1 to a circular shape. It is natural to assume that in d dimensions the n -faced cell will similarly tend to a hypersphere when $n \rightarrow \infty$. Let R denote the n dependent radius of this sphere. Then the central seed has its n first-neighbor seeds located, for large n , within a narrow spherical shell of radius $2R$. We denote the width of this shell by w ; approach to sphericity means that $w/R \rightarrow 0$ as $n \rightarrow \infty$.

This leads us to the ‘shell’ model for the first-order neighbor seeds represented in figure 1. We consider two d -dimensional hyperspheres of radii $2R$ and $2R - w$, both centered around the central seed. Let all seeds other than the central one be distributed independently and uniformly in space with density ρ . Let now $p_n(d; R, w)$ denote the probability of the event – which defines the ‘shell’ model – that (i) the inner hypersphere contains no other seeds than the central one; and (ii) the shell contains exactly n seeds. Our procedure will be to write $p_n(d; R, w)$ as an explicit function of n , d , and the two parameters R and w (this is easy). We will then, by means of a heuristic argument, express w in terms of R and finally maximize with respect to R . The result will be the desired expression for $p_n(d)$.

The probability $p_n(d; R, w)$ follows from an elementary calculation and is equal to

$$p_n(d; R, w) = \frac{(\rho V_1)^n}{n!} e^{-\rho V_2}, \quad (2.1)$$

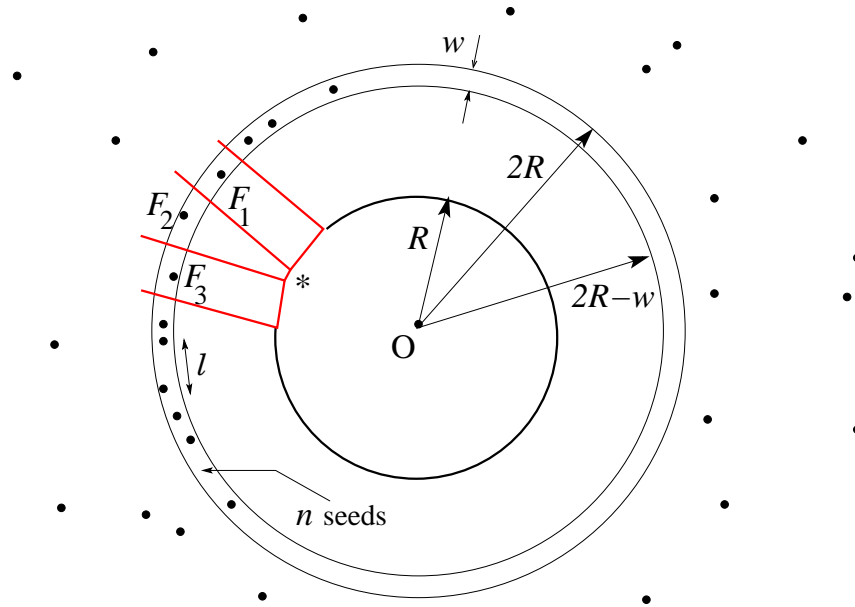


Figure 1: Schematic representation of the ‘shell’ model of the first-neighbor seeds. Two hyperspheres (of radii $2R$ and $2R - w$) are centered about the origin O of d -dimensional space. A ‘central’ seed is located in O . Other seeds are distributed randomly and uniformly with density ρ . The picture shows the rare event of having (i) n seeds inside the shell; (ii) no seed inside the inner hypersphere. The circle of radius R is the approximate boundary of the central Voronoi cell. The asterisk denotes the location of contact between the central cell and the cell of seed F_2 . Further explanation is given in the text.

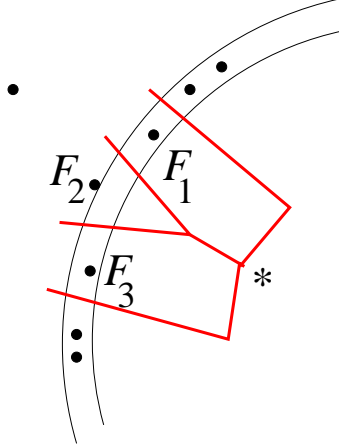


Figure 2: Detail of figure 1 in which seed F_2 has moved a little outward and is now screened by its neighbors F_1 and F_3 from being in contact with the central cell.

where $V_1(R, w)$ and $V_2(R)$ are the volumes of the shell and of the outer sphere, respectively. We will denote the volume v_d and the surface area s_d of the d -dimensional hypersphere of unit radius by

$$v_d = \pi^{\frac{d}{2}} / \left(\frac{d}{2}\right)!, \quad s_d = 2\pi^{\frac{d}{2}} / \left(\frac{d}{2} - 1\right)! \quad (2.2)$$

Therefore

$$\begin{aligned} V_1(R, w) &= v_d \left\{ (2R)^d - (2R - w)^d \right\}, \\ V_2(R) &= v_d (2R)^d. \end{aligned} \quad (2.3)$$

It will be convenient to work with $\log p_n$. Using (2.3) in (2.1) we find

$$\log p_n(d; R, w) = -\log n! - \log \left[\rho v_d \left\{ (2R)^d - (2R - w)^d \right\} \right] - \rho v_d (2R)^d, \quad (2.4)$$

which is exact within the shell model. This expression for $p_n(d; R, w)$ will be at the basis of what is to follow.

2.2 Relation between w and R

We now look for a relation between w and R . Figure 1 is a schematic two-dimensional representation of a d -dimensional situation. It shows part of the Voronoi cell boundaries of three first-order neighbor seeds F_1 , F_2 , and F_3 . Each line segment in the figure belongs to a $(d - 1)$ -dimensional face that perpendicularly bisects the line segment joining two neighboring seeds. An asterisk marks the short line segment common to the central cell and the cell

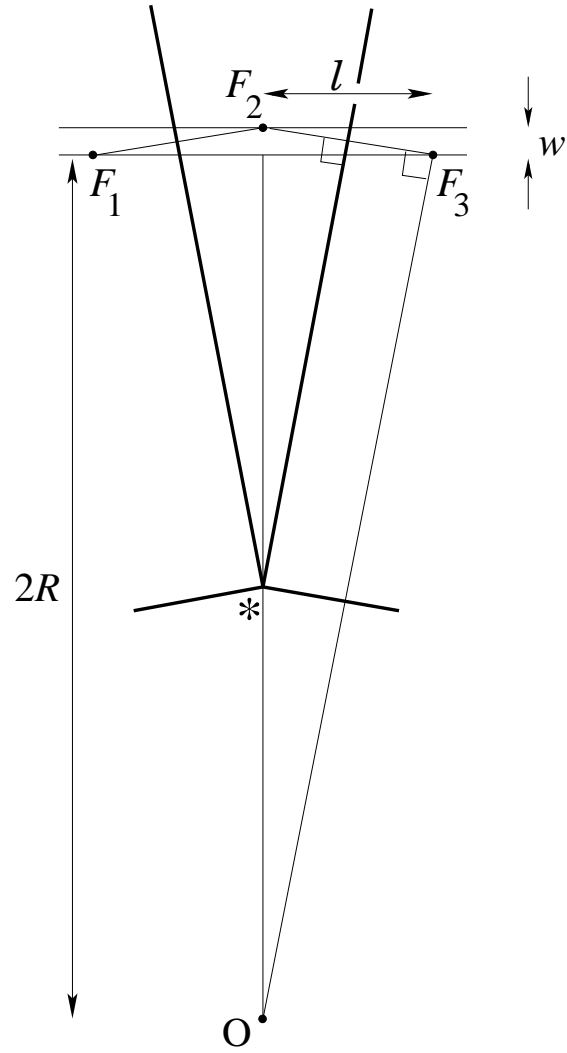


Figure 3: Marginal situation in between those of figures 1 and 2. The central cell has a point contact with the cell of seed F_2 in the four-vertex denoted by the asterisk.

of F_2 . As shown in figure 2, this face is so small that it disappears when F_2 , roughly speaking, crosses to the outside of the outer hypersphere: F_2 is then be ‘screened’ by its neighboring seeds F_1 and F_3 . When w is small with respect to the typical interseed distance ℓ in the shell, then such screening will be negligible for a random arrangement of the n seeds in the shell. We now relate shell width w to the radius R by imposing that w be small enough for this to be the case, but otherwise as large as possible. Figure 3 depicts a marginal situation in which the screening of F_2 by F_1 and F_3 sets in. The idealization consisting in placing F_1 and F_3 at equal distances from the origin and symmetrically with respect to F_2 is good enough for our purpose. Elementary geometry then shows that w , ℓ , and R are related by

$$\frac{w}{\ell} \sim \frac{\ell}{2R}. \quad (2.5)$$

where the symbol \sim denotes proportionality in the limit of large n . We now wish to eliminate ℓ from this relation.

The shell may be considered locally as a flat $(d-1)$ -dimensional space if

$$w \ll \ell \ll R. \quad (2.6)$$

We will assume here, and be able to verify afterwards, that in the limit of large n these conditions are satisfied. The typical interseed distance ℓ between the first-neighbor seeds in the shell is then easily found. For $w \ll \ell$ the n seeds may be considered as distributed on a $(d-1)$ -dimensional hypersurface of area

$$S = s_d(2R)^{d-1}. \quad (2.7)$$

They therefore have a $(d-1)$ -dimensional surface density $\sigma = n/S$, whence it follows that their typical distance ℓ may be defined by

$$v_{d-1}\ell^{d-1} = Sn^{-1}. \quad (2.8)$$

From (2.7) and (2.8) it follows that

$$\ell = 2R \left(\frac{s_d}{nv_{d-1}} \right)^{\frac{1}{d-1}}. \quad (2.9)$$

Comparing finally (2.9) and (2.5) suggests that in the shell model we should set

$$w = 2R(c_d n)^{-\frac{2}{d-1}}, \quad (2.10)$$

where c_d is a (not exactly known) numerical constant of order unity. Whereas we have argued above for the validity of (2.10) in the limit of asymptotically large n and R , we adopt it now as part of the definition of the shell model

for arbitrary w and R . At this point it may be verified that the necessary conditions (2.6) both hold if

$$(c_d n)^{-\frac{1}{d-1}} \ll 1. \quad (2.11)$$

Equation (2.10) is the desired relation between w and R .

2.3 Maximizing the entropy

Upon substituting (2.10) in (2.4) and denoting the result by $p_n(d; R)$ we obtain

$$\log p_n(d; R) = -\log n! + n \log \rho v_d (2R)^d - \rho v_d (2R)^d + n \log Z_n(d) \quad (2.12)$$

where

$$\begin{aligned} Z_n(d) &= 1 - \left\{ 1 - (c_d n)^{-\frac{2}{d-1}} \right\}^d \\ &\simeq d (c_d n)^{-\frac{2}{d-1}}, \end{aligned} \quad (2.13)$$

in which the second line represents the leading order behavior as $n \rightarrow \infty$.

Equation (2.12) represents the entropy of the arrangement of seeds and still contains R as a free parameter. It is again easy to maximize $\log p_n(d; R)$ expression with respect to R .

Upon varying the right hand side of (2.12) with respect to R we find that it has its maximum for $R = R_*$ where

$$2R_* = \left(\frac{n}{\rho v_d} \right)^{\frac{1}{d}}. \quad (2.14)$$

The corresponding w_* follows from substitution of (2.14) in (2.10). We are now ready to obtain our heuristic result as the probability that maximizes the configurational entropy, that is, $p_n(d) = p_n(d; R_*)$. Substitution of (2.14) and (2.13) in (2.12) yields

$$\log p_n(d) = -\log n! + n \log n - n + n \log \left[d (c_d n)^{-\frac{2}{d-1}} \right] + n \log z_n(d), \quad (2.15)$$

in which

$$\begin{aligned} \epsilon_n(d) &= d^{-1} (c_d n)^{\frac{2}{d-1}} Z_n(d) - 1 \\ &= \sum_{k=1}^{d-1} \frac{(-1)^k}{d} \binom{d}{k+1} (c_d n)^{-\frac{2k}{d-1}} \end{aligned} \quad (2.16)$$

is a polynomial in $(c_d n)^{-\frac{2}{d-1}}$ without constant term. This may be rearranged to yield the large- n expansion

$$\log p_n(d) = -\log \left[\left(\frac{2n}{d-1} \right)! \right] + n \log A_d + n \log [1 + \epsilon_n(d)] + \frac{1}{2} \log \frac{2}{d-1} + o(1), \quad (2.17)$$

where A_d is an abbreviation for

$$A_d = d \left[\frac{1}{2} (d-1) c_d e \right]^{-\frac{2}{d-1}}. \quad (2.18)$$

Hence we may write

$$p_n(d) = \left(\frac{2}{d-1} \right)^{\frac{1}{2}} \frac{A_d^n}{\left(\frac{2n}{d-1} \right)!} [1 + \epsilon_n(d)]^n [1 + o(1)], \quad n \rightarrow \infty, \quad (2.19)$$

which is our final result for general d .

Since $1 + \epsilon_n(d)$ has to be elevated to the n th power, this polynomial cannot be included with the $o(1)$ terms when $d > 3$. Dimension $d = 3$ is a marginal case and $\epsilon_n(3)$ contributes to the constant prefactor of $p_n(3)$. Hence $p_n(3)$ is given by

$$p_n(3) = C \frac{A_3^n}{n!} [1 + o(1)], \quad n \rightarrow \infty, \quad (2.20)$$

in which $C = \exp(-1/c_3)$ and $A_3 = 1/(3c_3 e)$ are numerical constants.

2.4 Comments

The arguments of this section are heuristic. Their validity is best assessed by a comparison to the two-dimensional case where exact results are available. These strongly suggest that the inverse factorial $1/\left(\frac{2n}{d-1}\right)!$, which is the dominant factor in the large- n behavior in (2.19) and (2.20), are exact. They also lead us to believe that the functional form of $p_n(d)$, that is, an exponential divided by a factorial, can be trusted. The value of the numerical constant c_d and hence of A_d remain, however, undetermined, since c_d appears in the theory only as a proportionality constant in the order-of-magnitude estimate (2.10). Finally, the decay of $p_n(d)$ with growing n is less fast than in dimension $d = 2$, where $p_n(2) \sim A_2^n/(2n)!$ as shown by (1.1).

3 Aboav's law in dimension $d = 3$

3.1 The plane \mathcal{F} of first neighbors

For large n the first-neighbor seeds are arranged in a nearly spherical shell. Its radius, according to (2.14) and (2.2), is equal to $2R_* = \frac{1}{4}(6n/\pi\rho)^{1/3}$ and its width, according to (2.14) and (2.10), is $w_* \sim (\rho n^2)^{-1/3}$. This width may be set to zero for all considerations of this section, which means neglecting the

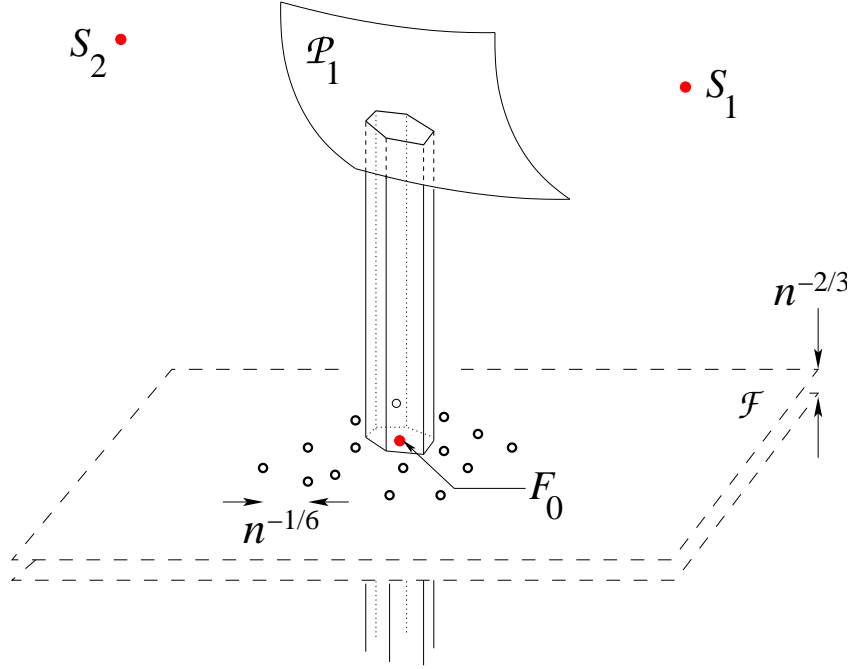


Figure 4: The plane \mathcal{F} , whose actual width $w_* \sim n^{-2/3}$ may be set to zero, contains the seeds that are first-neighbors to the central seed (the latter is located at a distance $2R_* \sim n^{1/3}$ below the plane and is not shown). S_1 and S_2 are second-neighbor seeds. \mathcal{P}_1 is the paraboloid of all points equidistant from S_1 and from \mathcal{F} . The ‘prism’ is the Voronoi cell of an arbitrarily selected first-neighbor seed F_0 . Each vertical face of this prism lies in a plane equidistant from a pair of points in \mathcal{F} . The intersection of the prism with \mathcal{F} is the boundary of the two-dimensional Voronoi cell of F_0 in \mathcal{F} . The prism intersects the parabola \mathcal{P}_1 according to a polygon which is the projection of this boundary. It defines the face that the Voronoi cells of F_0 and S_1 have in common. In the downward direction the Voronoi cell of F_0 ends by a face (not shown) in common with the central cell.

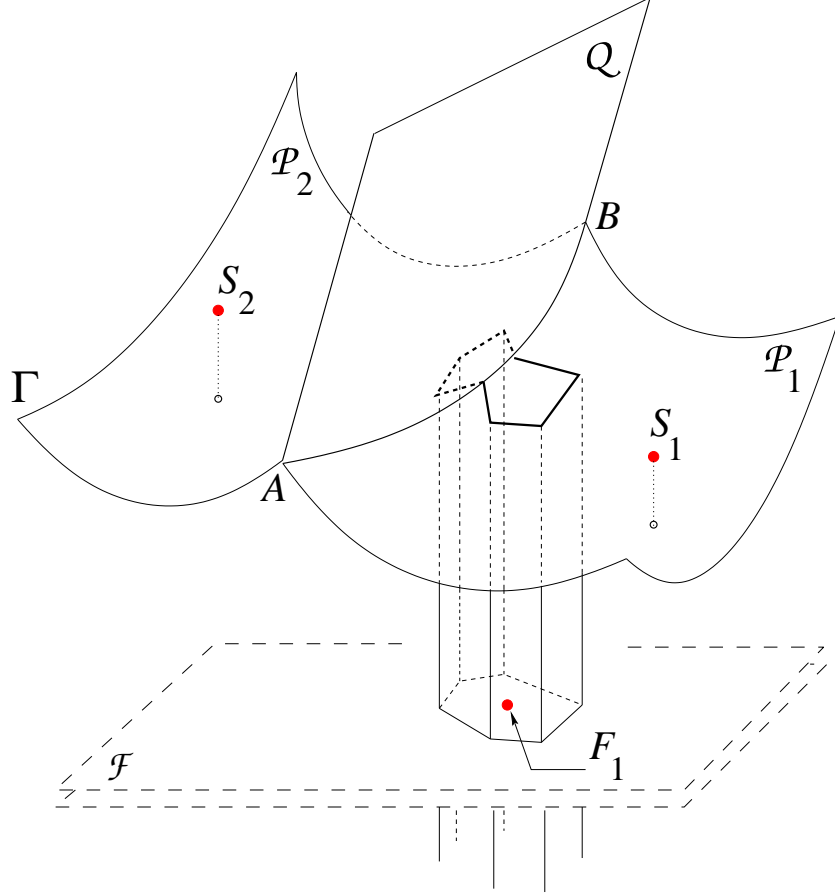


Figure 5: The piecewise paraboloidal surface Γ is the locus of points equidistant from the plane of first-neighbor seeds, \mathcal{F} , and the set of second-neighbor seeds $\{S_i\}$ constitutes a piecewise paraboloidal surface called Γ . All contributing paraboloids are circular and have their axes perpendicular to \mathcal{F} . In particular, \mathcal{P}_1 and \mathcal{P}_2 are the paraboloids of points equidistant from the seeds S_1 and S_2 , respectively, and the plane \mathcal{F} . The plane Q bisects the line segment S_1S_2 perpendicularly. The curved segment AB lies on the parabola along which \mathcal{P}_1 , \mathcal{P}_2 , and Q intersect. The Voronoi cell of the first-neighbor seed F_1 happens to intersect Γ at the intersection AB between two paraboloids. As a result this Voronoi cell has not one, but two faces at its upper end.

small random deviations of the radial coordinates of the first neighbors. The surface area of the sphere being $S = 4\pi(2R_*)^2 = \pi^{1/3}(6n/\rho)^{2/3}$, the typical interseed distance between the first-neighbor seeds is $\ell \sim (S/n)^{1/2} \sim (\rho^2 n)^{-1/6}$. On the scale of the interseed distances we may therefore consider the shell as a flat surface that we will denote by \mathcal{F} and also refer to as a ‘plane’. This situation has been represented in figure 4.

In the limit of large n the first-neighbor cells become very elongated prism-like objects, as already begins to be apparent in figure 1 (snapshots of realistic *two*-dimensional many-sided cells with n as high as 1500 are shown in reference [15]). Each first-neighbor cell has one face in common with the central cell. With the width of \mathcal{F} set to zero, the faces between adjacent first neighbors are perpendicular to \mathcal{F} and define the sides of a prism around each first neighbor. These prisms intersect the plane \mathcal{F} according to a two-dimensional cellular structure. The typical cell area in \mathcal{F} is $a = S/n \sim \ell^2 \sim (\rho^2 n)^{-1/3}$. The seeds are not uniformly (Poisson) distributed in \mathcal{F} but will effectively repel each other; nevertheless, just for topological reasons, the cells in the plane \mathcal{F} have an average of exactly six neighbors.

3.2 First and second neighbors

We consider now the faces between the first and second-neighbor cells. The second-neighbor seeds are marked S_1, S_2, \dots in figures 4 and 5. There is no restriction on their positions as long as they stay out of the sphere of radius $2R_*$, and the typical distance $\rho^{-1/3}$ between them is independent of n . We denote by Γ the surface of points that are equidistant from \mathcal{F} and from the set $\{S_i\}$ of second neighbors. Since for $n \rightarrow \infty$ the first-neighbor seeds become infinitely dense in \mathcal{F} , in that limit Γ is a piecewise paraboloidal surface. The paraboloids join along lines of intersection (‘seams’) that are segments of parabolas. For example, the curve AB in figure 5 lies on such a parabolic seam. For the considerations that follow it will be convenient to project Γ onto \mathcal{F} . The set of parabolic seams of Γ will project onto \mathcal{F} as a two-dimensional cellular net of trivalent vertices, connected by segments of parabolas. We will refer to the cells of this network as ‘supercells’ in order to distinguish them from the ‘ordinary’ cells (discussed above) due to the intersections of the prisms with \mathcal{F} . The typical supercell area will be of order $\sim n^0$ as $n \rightarrow \infty$. Since the radius of the spherical shell behaves as $R_* \sim n^{1/3}$, it is well approximated by the flat surface \mathcal{F} also at the scale of the supercells.

We analyze now, within the plane \mathcal{F} , the intersection of the net of supercells with the ordinary cells. In the limit $n \rightarrow \infty$ the fraction of ordinary cells *not* intersected by a segment of the supercell net will tend to unity. For reasons that will become clear just below we denote this fraction of ordinary cells by f_8 . The prism (three-dimensional cell) that encloses a cell of this

type, will therefore be bounded below by the central cell and above by a *single* second-neighbor cell. Since (for mere topological reasons) such cells are adjacent to, on average, six other first-neighbor cells, their total number of neighbors is eight.

There are, however, two special types of ordinary cells: (a) those intersected by a perimeter segment of a supercell; and (b) those containing the vertex where three such perimeter segments join. In figure 5 the cell of seed F_1 is an example of a special cell of type (a). These two special types of cells will represent fractions of all ordinary cells to be denoted f_9 and f_{10} , respectively. A counting similar to the one above easily shows that the corresponding types of three-dimensional cells have 9 and 10 neighbors, respectively.

For $n \rightarrow \infty$ the fractions f_9 and f_{10} will vanish, and we will now determine exactly how. Since the supercells are of linear dimension $\sim n^0$ and the ordinary cells of linear dimension $\sim n^{-1/6}$, a supercell will contain $\sim n^{1/3}$ ordinary cells. Only a finite number of these (on average six) will be located on the vertices of the supercell, and therefore we deduce that $f_{10} = a_2 n^{-1/3}$ as $n \rightarrow \infty$, where a_2 is a numerical constant. The parabolic segments of a supercell perimeter are straight lines at the scale of the ordinary cells. Typically such a perimeter segment will therefore intersect $\sim n^{1/6}$ ordinary cells. Hence f_9 is of order $n^{-1/6}$. Assuming an expansion in powers of $n^{-1/6}$ we will write $f_9 = a_1 n^{-1/6} + b_1 n^{-1/3}$, where a_1 and b_1 are numerical constants.

To order $n^{-1/3}$ we have that $f_8 + f_9 + f_{10} = 1$. Hence to this order the average number of neighbors $m_n(3)$ of a cell with n neighbors is given by

$$m_n(3) = 8f_8 + 9f_9 + 10f_{10}. \quad (3.1)$$

Substituting the above expressions for the f_n yields

$$m_n(3) = 8 + k_1 n^{-1/6} + k_2 n^{-1/3} + \dots, \quad (3.2)$$

in which $k_1 = a_1$ and $k_2 = b_1 + 2a_1$. The constants $k_1 > 0$ and k_2 are unknown. Equation (3.2) is the two-dimensional counterpart of (1.2). It shows that in dimension $d = 3$ Aboav's linear law *cannot hold* for n asymptotically large. This law therefore is necessarily an approximation (and possibly a very good one) in the experimentally accessible window of n values. Below we will study the deviation from Aboav's law numerically.

4 Comparison to simulation data

In the preceding sections we derived results that are asymptotic in n , whereas data are mostly in a certain range of small n . In earlier work it turned out [11], however, that the asymptotic expression for the nearest-neighbor correlation $m_n(2)$ gives a good approximation to the two-dimensional data for

all n values. We may therefore hope that equation (3.2) will similarly provide a good fit to the three-dimensional data. Only few such data exist. The ones most relevant are due to Kumar *et al.* [17]. These authors determined by simulation, among several other quantities, the probability $p_n(3)$ and the correlation $m_n(3)$ in the range $10 \leq n \leq 22$. Their $p_n(3)$ data, not shown here, peak at $n = 15$. We have reproduced their $m_n(3)$ data in our figure 6. Following Earnshaw and Robinson [18], we plot m_n as a function of $1/n$ (rather than m_n or nm_n as a function of n). In the m_n *versus* $1/n$ plot Aboav's law again corresponds to a straight line, but deviations from linearity are easier to detect.

Within the measurement window $m_n(3)$ is clearly seen to decrease with n , but only from around 16.4 to 16.1. Kumar *et al.* fitted this behavior by

$$m_n(3) = 16.57 - 0.02n, \quad (4.1)$$

represented by the dashed line in figure 6. This relation obviously cannot be asymptotic. In a later analysis of the same data, Fortes [19] proposed to fit them by Aboav's law, namely

$$m_n(3) = 15.95 + \frac{4.45}{n}. \quad (4.2)$$

It is shown as the straight dotted line in figure 6.

We wish to compare these two earlier fits to our theoretical functional form, equation (3.2). To that end we choose the constants k_1 and k_2 such that in $n = 15$ (where p_n is maximum) our curve and the dashed fit produce the same values of $m_n(3)$ and its n -derivative, that is, $m_{15}(3) = 16.27$ and $m'_{15}(3) = -0.02$. This leads to $k_1 = 23.15$ and $k_2 = -15.96$. The result is the solid curve shown in the figure. We emphasize that this procedure involves the additional assumption that it is correct in the finite- n regime to use the asymptotic expression (3.2) with all terms beyond order $n^{-1/3}$ discarded.

Returning now to figure 6, we observe that the simulation data scatter too much to be able to unambiguously distinguish between the three curves. The considerations of this section point to a most interesting question: can one establish by Monte Carlo simulation the presence of the downward curvature in the m_n *versus* $1/n$ plot in three dimensions? Curvature, although not proving (3.2), would at least rule out Aboav's law. Simulations at least an order of magnitude larger than the existing ones will be necessary; this however is within present-day machine capacity.

5 Conclusion

We have considered Poisson-Voronoi diagrams in spatial dimensions d higher than two. We obtained analytic expressions for (i) the facedness (or : neighbor number) probability $p_n(d)$ and (ii) the two-cell correlation $m_n(3)$, both

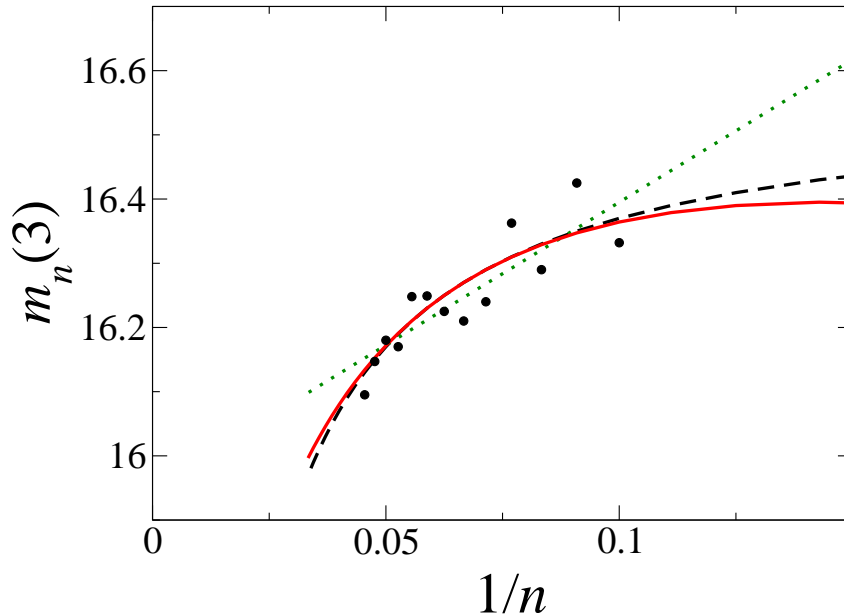


Figure 6: Dots: data points by Kumar *et al.* [17]. Straight dotted line: Aboav's law with parameters as in (4.2) due to Fortes [19]. Dashed curve : nonasymptotic fit (4.1) due to Kumar *et al.* Solid curve: our theoretical equation (3.2) for the values of k_1 and k_2 given in the text.

valid in the limit of asymptotically large n . We conclude that Aboav's law cannot be strictly valid in dimension $d = 3$, although it may be a very good approximation in the regime most easily accessible to experiment and simulation. These results rest on heuristic arguments developed in analogy to reasoning previously shown [9] to be valid in two dimensions. They cannot be considered as mathematically proved, but their value derives from the fact that this is the only theoretical work so far in this direction. We believe that confirmation of the failure of Aboav's law in three dimensions is within the reach of Monte Carlo simulations that are possible today.

References

- [1] A. Okabe, B. Boots, K. Sugihara, and S.N. Chiu, *Spatial tessellations: concepts and applications of Voronoi diagrams*, second edition (John Wiley & Sons Ltd., Chichester, 2000).
- [2] N. Rivier, in *Disorder and Granular Media*, eds. D. Bideaux and A. Hansen (Elsevier, Amsterdam 1993).
- [3] H.J. Hilhorst, *J. Stat. Mech.* P09005 (2005).

- [4] J.L. Meijering, *Philips Research Reports* **8**, 270 (1953).
- [5] J. Møller, *Adv. Appl. Prob.* **21**, 37 (1989).
- [6] J. Møller and D. Stoyan, *Stochastic Geometry and Random Tessellations* preprint 2007. To appear in: “Tessellations in the Sciences: Virtues, Techniques and Applications of Geometric Tilings”, eds. R. van de Weijgaert, G. Vegter, V. Icke, and J. Ritzerveld. Springer Verlag.
- [7] The value of $\langle n \rangle_4$ may be deduced from the relations given in Ref. [5].
- [8] H.J. Hilhorst, *J. Stat. Mech.* L02003 (2005).
- [9] H.J. Hilhorst, *J. Stat. Mech.* P05007 (2009).
- [10] D.A. Aboav, *Metallography* **3**, 383 (1970).
- [11] H.J. Hilhorst, *J. Phys. A* **39**, 7227 (2006).
- [12] B.N. Boots and D.J. Murdoch, *Computers and Geosciences* **9**, 351 (1983).
- [13] G. Le Caër and J. S. Ho, *J. Phys. A* **23**, 3297 (1990).
- [14] K.A. Brakke, unpublished.
Available on <http://www.susqu.edu/brakke/aux/downloads/200.pdf>.
- [15] H.J. Hilhorst, *J. Phys. A* **40**, 2615 (2007).
- [16] H.J. Hilhorst *European Physical Journal B* **64**, 437 (2008).
- [17] S. Kumar, S.K. Kurtz, J.R. Banavar, and M.G. Sharma, *J. Stat. Phys.* **67**, 523 (1992).
- [18] J.C. Earnshaw and J.D. Robinson, *Phys. Rev. Lett.* **72**, 3682 (1994).
- [19] M.A. Fortes, *Phil. Mag. Lett.* **68**, 69 (1993).